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The Effects of Electron Screening Length and Emitter Quasi-Bound States on the Polar-Optical Phonon Scattering in Resonant Tunneling Diodes

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Abstract

Polar optical phonon (POP) scattering is one of the dominant scattering mechanisms contributing to the valley current in GaAs and InP based resonant tunneling diodes (RTDs). We systematically explore two model parameters which determine the strength of the POP scattering enhanced valley current: (1) the electron screening length and (2) the length of the emitter electron accumulation region included in the simulation. When emitter quasi-bound states are included in the simulation, reasonable agreements with experiment can be obtained with screening lengths of 15–30nm.

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RTDs are presently developed for circuit applications such as low power memory cells [1], high speed adders [2], and high speed logic [3]. RTD device performance is ultimately limited by the amplitude of the off-resonant valley current due to incoherent scattering processes such as polar optical phonon (POP), acoustic phonon, interface roughness (IR) and alloy disorder scattering. The scattering mechanisms that give rise to valley currents in RTDs have been studied using a number of different approaches [4].

To aid quantitative quantum device design, we developed a comprehensive 1-D device simulator called NEMO (Nanoelectronic Modeling) [5]. Our approach is based on a non-equilibrium Green function formalism which includes scattering effects through self-energy terms in a truncated self-consistent Born approximation [6]. This algorithm is similar to the multiple sequential scattering algorithm described by Roblin and Liou [4b]. We model interface roughness as a single layer of alloy where the cations of a single species cluster into islands [6,7]. A screened bulk Fröhlich Hamiltonian is used to model the POP interaction [6]. Since the self-energies have a strong momentum dependence, we numerically integrate over the incident transverse momenta.

In this study, we compare our I–V simulations with experimentally measured I–Vs for a GaAs-AlAs RTD device. Prior calculations using bulk phonons typically assumed an unscreened potential [4a,b]. Here, we include screening effects and investigate the dependence of the RTD electron density and valley current on the the screening length.

We also investigate the calculation accuracy as a function of a key simulation construct referred to as the non-equilibrium region. To enhance the calculation speed, NEMO allows the user to limit the electron transport and incoherent scattering calculation to a non-equilibrium region that extends over a portion of the device [6]. Portions of the device located outside the non-equilibrium region are treated as reservoirs in a local equilibrium characterized by a separate Quasi-Fermi level. To reduce the computational burden, we want to minimize the non-equilibrium region without sacrificing the accuracy of the calculation. This study determines the optimum location and extent of the non-equilibrium region for this calculation. The minimum extent in the simulations presented here is the central RTD device region (0-13nm). The spatial coordinate system in Figure (1) is shifted such that 0 coincides with the last site in the emitter region (adjacent to the left barrier).

The GaAs-AlAs RTD used for this comparison was grown by molecular-beam-epitaxy with 19.5 nm intrinsic GaAs spacer layers, 3.1 nm AlAs barriers, and a 6.2 nm GaAs well. The n^+ contacts are Si doped at 10^{18} cm^{-3}. Measurements are made at a temperature of 4.2 K to eliminate tunneling through X states in the AlAs barriers.

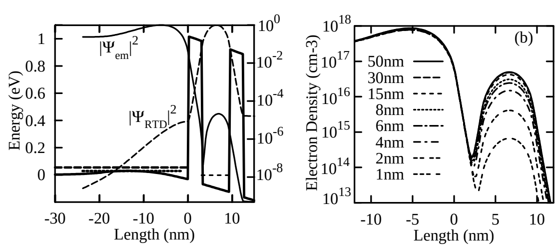

FIG. 1. (a) Left scale: Conduction band edge, resonance levels, and emitter Fermi energy (54 meV) of the RTD at a bias of 0.41V. The RTD ground state is indicated at an energy -0.18 meV and the emitter quasi bound state is indicated at 28 meV. Right Scale: $|\Psi(x)|^2$ for the emitter quasi-bound state and the RTD ground state. (b) Electron density calculated with scattering due to polar optical phonons for various electron screening lengths.

Figure (1a) shows the conduction band edge, the resonance levels, and the emitter Fermi level of our sample device at a bias of 0.41V (corresponding to the peak of the phonon-peak in the valley current). A no-scattering calculation indicates that the emitter quasi-bound state lies fully within in the Fermi sea at an energy of 28 meV. The RTD ground state has an energy of -0.18meV [8].

Figure (1b) shows a plot of the electron density calculated with polar optical phonon scattering for various electron screening lengths at a bias of 0.41V. The non-equilibrium region extends 12 nm into the emitter. The calcuation indicates a strong dependence of well occupation on the electron screening length.

Figure (2) shows the valley current dependence on the electron screening length for two different non-equilibrium region lengths: the minimal RTD region (0...13nm, labeled from now on I=0nm) and a region including the emitter quasi-bound state (-17...13nm, labeled I=17nm). Both cases show that the valley current increasing dramatically with screening length while the phonon peak shifts moderately to higher voltage. This effect is especially strong in the I=0 nm case in Figure (2a). We attribute this shift to the strong dependence of the POP scattering self-energy on the screening length, which alters the resonance spectrum in the RTD.

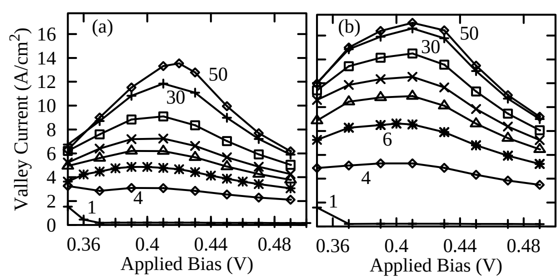

FIG. 2. POP scattering enhanced valley current for various screening lengths (50, 30, 15, 10, 8, 6, 4, and 1 nm). (a) Minimal non-equilibrium region (0...13nm) (I=0nm) (b) Broad non-equilibrium region (-17...13nm) (I=17nm).

The calculated valley current should become constant for a sufficiently large non-equilibrium region. To illustrate this, Figure (3a) plots the valley current at 0.41 V as a function of interaction region length for a variety of screening lengths. The valley current saturates for interaction region lengths of 10-15 nm. At this length, the non-equilibrium fully includes the emitter bound state. Any additional contributions to the overlap of the emitter quasi-bound state and the central RTD state are decaying exponentially as shown in Figure (1a). We attribute non-monotonic behavior at low interaction region lengths to the shift in the phonon peak as discussed with Figure (2). Figure (3b) contains the points in (3a) normalized to the saturation values. The non-equilibrium region must extend over the quasi-bound emitter state before the valley current becomes independent of the screening length. For short screening lengths (1 and 2 nm), we can obtain a saturated valley current at non-equilibrium region lengths greater than 5nm.

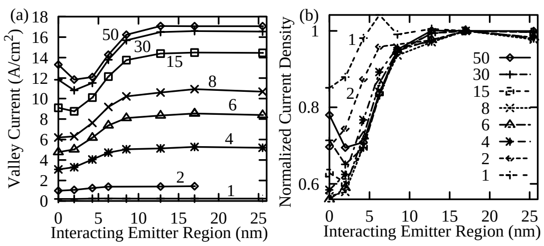

FIG. 3. (a) POP scattering enhanced valley current as a function of non-equilibrium emitter region length at *one* bias of 0.41 for various screening lengths (50, 30, 15, 8, 6, 4, 2, and 1 nm). (b) Same as (a) normalized to the saturation value at the longest interaction length.

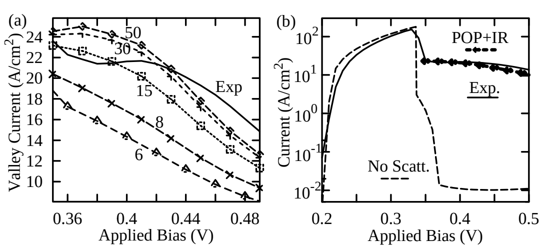

FIG. 4. (a) Valley current for POP scattering with various electron screening lengths and IR scattering compared to experiment. (b) Experimental current voltage characteristic on a logarithmic scale compared to a no scattering simulation and the valley current simulation with POP (15 nm screening length, 17 nm non-equilibrium emitter region) and IR scattering (10 nm correlation length).

To match the amplitude of the valley current with the experimental data, we included interface roughness [6,7] (IR) scattering into the simulation. Figure (4) shows the valley current calculated for various electron screening lengths using a non-equilibrium region extending to -17 nm and an exponential interface roughness correlation of length 10 nm. The inclusion of interface roughness scattering increases the valley current by 4 orders of magnitude to a level comparable to the experimental measurement.

To summarize, we have explored the dependence of the valley current on the electron screening length and the non-equilibrium region length. We find that the non-equilibrium region should include emitter quasi-bound states and that reasonable screening lengths of 15 nm can provide scattering to match the valley current of our GaAs/AlGaAs RTD.

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[8] The resonance energies will be modified by several meV due to the scattering selfenergies.